10670105 HydroformylationEthyUnsatCmp 407578-79-4

=> s 407578-79-4/rn
L7 1 407578-79-4/RN

=> fil hcap
COST IN U.S. DOLLARS SINCE FILE ENTRY 0.45 TOTAL SESSION 72.51

FULL ESTIMATED COST

FILE 'HCAPLUS' ENTERED AT 14:34:29 ON 19 FEB 2007
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FILE COVERS 1907 - 19 Feb 2007 VOL 146 ISS 9
FILE LAST UPDATED: 18 Feb 2007 (20070218/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l7
L8 3 L7

=> d ibib abs l8 1-3

L8 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:141010 HCAPLUS
DOCUMENT NUMBER: 142:221614
TITLE: Carbonylation of conjugated dienes using palladium-phosphine complex catalysts with improved stability
INVENTOR(S): Sielcken, Otto Erik; Baur, Henricus Anna Christiaan; Toth, Imre
PATENT ASSIGNEE(S): DSM IP Assets B. V., Neth.
SOURCE: PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005014520	A1	20050217	WO 2004-EP7059	20040628

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,

GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
SN, TD, TG

EP 1656336	A1	20060517	EP 2004-740443	20040628
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1829679	A	20060906	CN 2004-80021621	20040628
PRIORITY APPLN. INFO.:			EP 2003-77340	A 20030725 X
			WO 2004-EP7059	W 20040628

OTHER SOURCE(S): CASREACT 142:221614; MARPAT 142:221614

AB A process for carbonylation of a conjugated diene is carried out by reacting the conjugated diene with carbon monoxide and a hydroxyl group-containing compound in the presence of a palladium catalyst system in a reaction zone to produce a reaction mixture, the catalyst system comprising (a) a source of palladium cations, (b) a mono-, bi- or multidentate phosphine ligand, containing at least one phosphorus atom directly bound to two or three aliphatic carbon atoms, as a process ligand to produce a palladium-phosphine ligand complex catalyst, and (c) a source of anions selected from carboxylic acid and halide ions. The process ligand (b) contains a moiety of the formula X-P(A1)(A2), where A1 and A2 each represent an aliphatic carbon atom which may be connected to one or more aliphatic or aromatic carbon atoms or both A1 and A2 may be a part of at least 5-membered ring including the phosphorus atom, and X represents an aliphatic or aromatic carbon atom which may be connected to one or more aliphatic or aromatic carbon atoms or X is a part of an organic bridging group connecting another identically or differently substituted phosphorus atom, the process ligand being fed continuously or periodically to the process as a ligand make-up at a temperature ≤ 50°. The catalysts have improved stability to degradation during the reaction and can be efficiently regenerated and in-process recycled. Thus, a homogeneous catalyst was prepared by dissolving under nitrogen palladium acetate (370 mg), 2,3-bis(9-phosphabicyclononyl)butane (589 mg) and pivalic acid (1.96 g) in freshly distilled Me pentenoates (98.9 g), and adding 21.6 μL of a 57%-aqueous hydrogen iodide. The catalyst showed selectivity of 87% after 86 h of use in a continuous carbonylation of butadiene into Me pentenoates carried out at 135° with parallel feeding of carbon monoxide, butadiene, the catalyst solution, and methanol, addnl. methanol solns. of 2,3-bis(9-phosphabicyclononyl)butane (166 mg/L) and pivalic acid (35 g/L) being fed into the catalyst feed line at room temperature

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	2004:287803 HCAPLUS
DOCUMENT NUMBER:	140:310272
TITLE:	Process for the hydroformylation of an ethylenically unsaturated compound
INVENTOR(S):	Drent, Eit; Van Ginkel, Roelof; Jager, Willem Wabe
PATENT ASSIGNEE(S):	Shell Internationale Research Maatschappij B.V., Neth.
SOURCE:	PCT Int. Appl., 28 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent

Just App

10670105 HydroformylationEthyUnsatCmp 407578-79-4

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004028689	A2	20040408	WO 2003-EP50654	20030924
WO 2004028689	A3	20040729		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2500095	A1	20040408	CA 2003-2500095	20030924
AU 2003299066	A1	20040419	AU 2003-299066	20030924
US 2004167362	A1	20040826	US 2003-670105	20030924
EP 1542798	A2	20050622	EP 2003-798198	20030924
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1684769	A	20051019	CN 2003-823006	20030924
JP 2006500415	T	20060105	JP 2004-539074	20030924
ZA 2005002080	A	20050912	ZA 2005-2080	20050311
PRIORITY APPLN. INFO.:			EP 2002-256696 A	20020926
			WO 2003-EP50654 W	20030924

OTHER SOURCE(S): MARPAT 140:310272

AB The present invention relates to a process for the hydroformylation of an optionally substituted ethylenically unsatd. compound by reaction thereof with carbon monoxide and hydrogen in the presence of a specific catalyst system. The specific catalyst system comprises (A) a source of group VIII metal cations, (B) a diphosphine ligand having the general formula X1RX2, (C) an acid with pKa < 3, measured in an aqueous solution at 18° or a salt derived thereof, and (D) a source of halide anions, wherein X1, X2 = independently an optionally substituted cyclic group with ≥5 ring atoms, of which one is a phosphorus atom, and R = a bivalent optionally substituted bridging group, connected to each phosphorus atom by a sp2 hybridized carbon atom. Furthermore some specific bidentate diphosphines used in this process are described. Thus, 1,2-dibromobenzene 9.44, 1,4-diazabicyclo[2,2,2]octane 22.4, 9-phosphabicyclo[3.3.1]nonane 13.0, and tetrakis(triphenylphosphine)palladium 2.32 g were heated at 140° to give 7.10 g (yield 50%) 1,2-bis(9-phosphabicyclo[3.3.1]nonyl)benzene, 0.40 mmol of which was mixed with methane sulfonic acid 1.0, hydrochloric acid 0.20, and palladium acetate 0.25 mmol, and 20 mL 1-octene and heated at 120° for 5 h under 20 bar carbon monoxide and 40 bar hydrogen to give an alkanol product >99, a linear alkanol product 68, and a hydrogenation product <1%.

L8 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:256216 HCAPLUS
DOCUMENT NUMBER: 136:296537
TITLE: Process and palladium-diphosphine catalyst system for the carbonylation of conjugated dienes
INVENTOR(S): Drent, Eit; Jager, Willem Wabe; Sielcken, Otto Erik; Toth, Imre
PATENT ASSIGNEE(S): DSM N.V., Neth.

10670105 HydroformylationEthyUnsatCmp 407578-79-4

SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002026690	A1	20020404	WO 2001-NL709	20010926
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002011067	A5	20020408	AU 2002-11067	20010926
EP 1332124	A1	20030806	EP 2001-979078	20010926
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US 2004039226	A1	20040226	US 2003-381040	20030825
US 6835850	B2	20041228		

PRIORITY APPLN. INFO.:

EP 2000-203355	A	20000927
EP 2000-203356	A	20000927
EP 2000-2000203355	A	20000927
EP 2000-2000203356	A	20000927
WO 2001-NL709	W	20010926

OTHER SOURCE(S): MARPAT 136:296537

AB Conjugated dienes (e.g., 1,3-butadiene) are readily subjected to carbonylation to produce unsatd. esters (e.g., Me 3-pentenoate which is an adipate ester precursor) by reacting the conjugated diene with carbon monoxide and an hydroxyl group-containing compound (e.g., methanol) in the presence of a catalyst system based on: (a) a source of palladium cations (e.g., palladium acetate); (b) a diphosphine ligand X1RX2 (X1, X2 = cyclic group with at least 5 ring atoms of which one is a phosphorus atom; R = bivalent aliphatic bridging group, connecting both phosphorus atoms containing from 2 to 4 atoms in the bridge which is substituted with at least one substituent, Ph group with both phosphorus groups bound to the 1,2-position); and (c) a source of anions (e.g., pivalic acid).

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 14:28:12 ON 19 FEB 2007)

FILE 'HCAPLUS' ENTERED AT 14:28:22 ON 19 FEB 2007
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FILE 'REGISTRY' ENTERED AT 14:29:00 ON 19 FEB 2007
L2 0 S L1

FILE 'HCAPLUS' ENTERED AT 14:29:41 ON 19 FEB 2007
E US20040167362/PN,PRN,AN

10670105 HydroformylationEthyUnsatCmp 407578-79-4

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L3              1 S E3

     FILE 'REGISTRY' ENTERED AT 14:31:23 ON 19 FEB 2007
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L5              1 S  676992-18-0/RN

     FILE 'HCAPLUS' ENTERED AT 14:33:07 ON 19 FEB 2007
L6              1 S L5

     FILE 'REGISTRY' ENTERED AT 14:34:18 ON 19 FEB 2007
L7              1 S  407578-79-4/RN

     FILE 'HCAPLUS' ENTERED AT 14:34:29 ON 19 FEB 2007
L8              3 S L7
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10670105 HydroformylationEthyUnsatCmp 676992-15-7

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L9 1 676992-15-7/RN

=> file hcap
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.45 99.65

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION
CA SUBSCRIBER PRICE 0.00 -2.34

FILE 'HCAPLUS' ENTERED AT 14:38:42 ON 19 FEB 2007
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FILE COVERS 1907 - 19 Feb 2007 VOL 146 ISS 9
FILE LAST UPDATED: 18 Feb 2007 (20070218/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l9
L10 2 L9

=> d ibib abs l10 1-2

L10 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:473316 HCAPLUS
DOCUMENT NUMBER: 145:145808
TITLE: Highly Selective Halide Anion-Promoted Palladium-Catalyzed Hydroformylation of Internal Alkenes to Linear Alcohols
AUTHOR(S): Konya, Denes; Lenero, Karina Q. Almeida; Drent, Eite
CORPORATE SOURCE: Shell Global Solutions, Amsterdam, 1030BN, Neth.
SOURCE: Organometallics (2006), 25(13), 3166-3174
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:145808
AB The authors report on their study of the Pd-catalyzed hydroformylation of alkenes. A (bcope)Pd(OTf)2 complex [bcope = 1,2-bis[(cyclooctyl)phosphino]ethane] with sub-stoichiometrically added halide

anions is a highly efficient homogeneous catalyst (precursor) to selectively convert internal linear alkenes into predominantly linear (detergent) alcs. under mild conditions. Halide anion-dependent effects on the hydroformylation reaction rate as well as its chemo- and regioselectivity are observed Thus, the rate of hydroformylation of thermally equilibrated internal higher alkenes increases by a factor of .apprx.6-7 with chloride/bromide and about a factor 3-4 with iodide, while the selectivity toward alcs. increases to almost 100% upon addition of a substoichiometric quantity (with respect to Pd) of the halide anion source. Curiously, the regioselectivity toward linear alc. increases in the reverse order, i.e., iodide > bromide > chloride. From a detailed anal. of the products obtained with model substrates, hydrogenolysis of (bcope)palladium-acyl intermediates is strongly accelerated by the presence of halide anions. From a comparison of the catalytic performance with some related L2Pd(OTf)2 complexes, in which L2 are bidentate phosphines closely related to bcope, it also appears that the ligand plays a critical role in the promoting effect of halide anions.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:287803 HCAPLUS
DOCUMENT NUMBER: 140:310272
TITLE: Process for the hydroformylation of an ethylenically unsaturated compound
INVENTOR(S): Drent, Eit; Van Ginkel, Roelof; Jager, Willem Wabe
PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B.V., Neth.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004028689	A2	20040408	WO 2003-EP50654	20030924
WO 2004028689	A3	20040729		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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AU 2003299066	A1	20040419	AU 2003-299066	20030924
US 2004167362	A1	20040826	US 2003-670105	20030924
EP 1542798	A2	20050622	EP 2003-798198	20030924
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1684769	A	20051019	CN 2003-823006	20030924
JP 2006500415	T	20060105	JP 2004-539074	20030924
ZA 2005002080	A	20050912	ZA 2005-2080	20050311

PRIORITY APPLN. INFO.: EP 2002-256696 A 20020926
WO 2003-EP50654 W 20030924

10670105 HydroformylationEthyUnsatCmp 676992-15-7

OTHER SOURCE(S): MARPAT 140:310272

AB The present invention relates to a process for the hydroformylation of an optionally substituted ethylenically unsatd. compound by reaction thereof with carbon monoxide and hydrogen in the presence of a specific catalyst system. The specific catalyst system comprises (A) a source of group VIII metal cations, (B) a diphosphine ligand having the general formula X1RX2, (C) an acid with pKa < 3, measured in an aqueous solution at 18° or a salt derived thereof, and (D) a source of halide anions, wherein X1, X2 = independently an optionally substituted cyclic group with ≥5 ring atoms, of which one is a phosphorus atom, and R = a bivalent optionally substituted bridging group, connected to each phosphorus atom by a sp2 hybridized carbon atom. Furthermore some specific bidentate diphosphines used in this process are described. Thus, 1,2-dibromobenzene 9.44, 1,4-diazabicyclo[2,2,2]octane 22.4, 9-phosphabicyclo[3.3.1]nonane 13.0, and tetrakis(triphenylphosphine)palladium 2.32 g were heated at 140° to give 7.10 g (yield 50%) 1,2-bis(9-phosphabicyclo[3.3.1]nonyl)benzene, 0.40 mmol of which was mixed with methane sulfonic acid 1.0, hydrochloric acid 0.20, and palladium acetate 0.25 mmol, and 20 mL 1-octene and heated at 120° for 5 h under 20 bar carbon monoxide and 40 bar hydrogen to give an alkanol product >99, a linear alkanol product 68, and a hydrogenation product <1%.

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FILE 'HCAPLUS' ENTERED AT 14:28:22 ON 19 FEB 2007
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FILE 'REGISTRY' ENTERED AT 14:29:00 ON 19 FEB 2007
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FILE 'HCAPLUS' ENTERED AT 14:29:41 ON 19 FEB 2007
E US20040167362/PN,PRN,AN
L3 1 S E3

FILE 'REGISTRY' ENTERED AT 14:31:23 ON 19 FEB 2007
L4 0 S E1-E12
L5 1 S 676992-18-0/RN

FILE 'HCAPLUS' ENTERED AT 14:33:07 ON 19 FEB 2007
L6 1 S L5

FILE 'REGISTRY' ENTERED AT 14:34:18 ON 19 FEB 2007
L7 1 S 407578-79-4/RN

FILE 'HCAPLUS' ENTERED AT 14:34:29 ON 19 FEB 2007
L8 3 S L7

FILE 'REGISTRY' ENTERED AT 14:38:30 ON 19 FEB 2007
L9 1 S 676992-15-7/RN

FILE 'HCAPLUS' ENTERED AT 14:38:42 ON 19 FEB 2007
L10 2 S L9

10670105 HydroformylationEthyUnsatCmp 676992-16-8

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L11 1 676992-16-8/RN

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FULL ESTIMATED COST 0.45 116.16

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION
CA SUBSCRIBER PRICE 0.00 -3.90

FILE 'HCAPLUS' ENTERED AT 14:41:16 ON 19 FEB 2007
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FILE COVERS 1907 - 19 Feb 2007 VOL 146 ISS 9
FILE LAST UPDATED: 18 Feb 2007 (20070218/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L12 1 L11

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L12 1 ANSWERS HCAPLUS COPYRIGHT 2007 ACS on STN
IC ICM B01J031-24
ICS B01J027-08; B01J031-02; C07F009-6568; C07F015-00; C07C045-50
CC 67-1 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 23
TI Process for the hydroformylation of an ethylenically unsaturated compound
ST process hydroformylation ethylenically unsatd compd; bisphosphabicyclononylbenzene ligand palladium acetate catalyst octene hydroformylation
IT Alkenes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(C11-12; hydroformylation of ethylenically unsatd. compds.)
IT Ligands
RL: CAT (Catalyst use); USES (Uses)
(bidentate, diphosphines, hydroformylation catalyst ligand; hydroformylation of ethylenically unsatd. compds.)
IT Hydroformylation

10670105 HydroformylationEthyUnsatCmp 676992-16-8

(hydroformylation of ethylenically unsatd. compds.)
IT Group VIII elements
RL: CAT (Catalyst use); USES (Uses)
(hydroformylation of ethylenically unsatd. compds.)
IT Catalysts
(hydroformylation; hydroformylation of ethylenically unsatd. compds.)
IT 676992-18-0 676992-19-1
RL: CAT (Catalyst use); USES (Uses)
(hydroformylation catalyst ligand; hydroformylation of ethylenically unsatd. compds.)
IT 407578-79-4P, 9-Phosphabicyclo[3.3.1]nonane, 9,9'-(1,2-phenylene)bis-
676992-15-7P 676992-16-8P
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(hydroformylation catalyst ligand; hydroformylation of ethylenically unsatd. compds.)
IT 3375-31-3
RL: CAT (Catalyst use); USES (Uses)
(hydroformylation of ethylenically unsatd. compds.)
IT 4547-43-7P, Hexanoic acid, 6-hydroxy-, methyl ester 167707-57-5P,
Pentanoic acid, 5-hydroxy-4-methyl-, methyl ester 676992-17-9P
RL: IMF (Industrial manufacture); PREP (Preparation)
(hydroformylation of ethylenically unsatd. compds.)
IT 111-66-0, 1-Octene 630-08-0, Carbon monoxide, reactions 818-59-7
1333-74-0, Hydrogen, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydroformylation of ethylenically unsatd. compds.)
IT 583-53-9, 1,2-Dibromobenzene 3141-26-2, 3,4-Dibromothiophene
13887-02-0, 9-Phosphabicyclo[3.3.1]nonane 75415-78-0,
1,2-Dibromocyclopentene
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant in hydroformylation catalyst ligand preparation; hydroformylation of ethylenically unsatd. compds.)

ALL ANSWERS HAVE BEEN SCANNED

=> dis his

(FILE 'HOME' ENTERED AT 14:28:12 ON 19 FEB 2007)

FILE 'HCAPLUS' ENTERED AT 14:28:22 ON 19 FEB 2007
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FILE 'REGISTRY' ENTERED AT 14:29:00 ON 19 FEB 2007
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FILE 'HCAPLUS' ENTERED AT 14:29:41 ON 19 FEB 2007
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FILE 'REGISTRY' ENTERED AT 14:31:23 ON 19 FEB 2007
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L5 1 S 676992-18-0/RN

FILE 'HCAPLUS' ENTERED AT 14:33:07 ON 19 FEB 2007
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10670105 HydroformylationEthyUnsatCmp 676992-16-8

FILE 'REGISTRY' ENTERED AT 14:34:18 ON 19 FEB 2007
L7 1 S 407578-79-4/RN

FILE 'HCAPLUS' ENTERED AT 14:34:29 ON 19 FEB 2007
L8 3 S L7

FILE 'REGISTRY' ENTERED AT 14:38:30 ON 19 FEB 2007
L9 1 S 676992-15-7/RN

FILE 'HCAPLUS' ENTERED AT 14:38:42 ON 19 FEB 2007
L10 2 S L9

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L11 1 S 676992-16-8/RN

FILE 'HCAPLUS' ENTERED AT 14:41:16 ON 19 FEB 2007
L12 1 S L11

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10670105 HydroformylationEthyUnsatCmp 676992-19-1

=> s 676992-19-1/rn
L13 1 676992-19-1/RN

=> fil hcap
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.45 124.41

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION
CA SUBSCRIBER PRICE 0.00 -3.90

FILE 'HCAPLUS' ENTERED AT 14:43:03 ON 19 FEB 2007
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FILE COVERS 1907 - 19 Feb 2007 VOL 146 ISS 9
FILE LAST UPDATED: 18 Feb 2007 (20070218/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l13
L14 1 L13

=> d ibib abs l14 1

L14 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:287803 HCAPLUS
DOCUMENT NUMBER: 140:310272
TITLE: Process for the hydroformylation of an ethylenically unsaturated compound
INVENTOR(S): Drent, Eit; Van Ginkel, Roelof; Jager, Willem Wabe
PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B.V., Neth.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004028689	A2	20040408	WO 2003-EP50654	20030924

10670105 HydroformylationEthyUnsatCmp 676992-19-1

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     WO 2004028689         A3     20040729
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
             GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
             LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
             OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
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     AU 2003299066         A1     20040419    AU 2003-299066         20030924
     US 2004167362         A1     20040826    US 2003-670105         20030924
     EP 1542798            A2     20050622    EP 2003-798198         20030924
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     CN 1684769            A      20051019    CN 2003-823006         20030924
     JP 2006500415         T      20060105    JP 2004-539074         20030924
     ZA 2005002080         A      20050912    ZA 2005-2080           20050311
PRIORITY APPLN. INFO.:                         EP 2002-256696      A  20020926
                                               WO 2003-EP50654     W  20030924

OTHER SOURCE(S):          MARPAT 140:310272
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AB The present invention relates to a process for the hydroformylation of an optionally substituted ethylenically unsatd. compound by reaction thereof with carbon monoxide and hydrogen in the presence of a specific catalyst system. The specific catalyst system comprises (A) a source of group VIII metal cations, (B) a diphosphine ligand having the general formula X1RX2, (C) an acid with pKa < 3, measured in an aqueous solution at 18° or a salt derived thereof, and (D) a source of halide anions, wherein X1, X2 = independently an optionally substituted cyclic group with ≥5 ring atoms, of which one is a phosphorus atom, and R = a bivalent optionally substituted bridging group, connected to each phosphorus atom by a sp2 hybridized carbon atom. Furthermore some specific bidentate diphosphines used in this process are described. Thus, 1,2-dibromobenzene 9.44, 1,4-diazabicyclo[2,2,2]octane 22.4, 9-phosphabicyclo[3.3.1]nonane 13.0, and tetrakis(triphenylphosphine)palladium 2.32 g were heated at 140° to give 7.10 g (yield 50%) 1,2-bis(9-phosphabicyclo[3.3.1]nonyl)benzene, 0.40 mmol of which was mixed with methane sulfonic acid 1.0, hydrochloric acid 0.20, and palladium acetate 0.25 mmol, and 20 mL 1-octene and heated at 120° for 5 h under 20 bar carbon monoxide and 40 bar hydrogen to give an alkanol product >99, a linear alkanol product 68, and a hydrogenation product <1%.

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L13            1 S 676992-19-1/RN

     FILE 'HCAPLUS' ENTERED AT 14:43:03 ON 19 FEB 2007
L14            1 S L13

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10670105 HydroformylationEthyUnsatCmp claim 11

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E US20040167362/PN,PRN,AN
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E US20040167362/PN,PRN,AN
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L5 1 S 676992-18-0/RN

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L13 1 S 676992-19-1/RN

FILE 'HCAPLUS' ENTERED AT 14:43:03 ON 19 FEB 2007
L14 1 S L13

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L16 0 S L15
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L17 0 S "BENZENE 1,2-P,P'BIS(9-PHOSPHABICYCLONONYL"/CN

10670105 HydroformylationEthyUnsatCmp claim 11

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L23           0 S "THIOPHENE, 3,4-P,P'BIS(9-PHOSPHABICYCLONONYL"/CN

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L24           0 S L23
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